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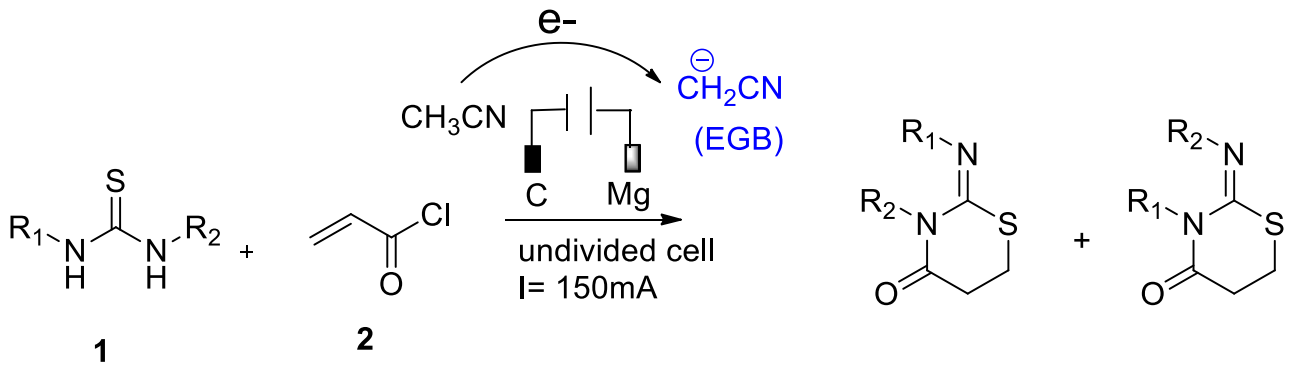
EFFICIENT SYNTHESIS OF IMINO-1,3-THIAZINAN-4-ONE PROMOTED BY ACETONITRILE ELECTROGENERATED BASE AND COMPUTATIONAL STADIES WITH CB1 AND 11 βHSD1 MOLECULES*

Keywords: *N,N′*-disubstituted thioureas, electrogenerated base, imino-1,3-thiazinan-4-one, organic acryloyl chloride, molecular docking, molecular Dynamics, DFT.

Currently, the search for compounds possessing medicinal activities is of special interest, especially the six membered ring compounds which are showed an interesting pharmaceutic activities, such as the thioxopyrimidinones which is used as anti-allergic and anti-cancer [1].

We are focused our attention here for the synthesis of six membered imino-1,3-thiazinan-4-one which is a substrate attracting attention as a novel therapeutic agent that stops or slows the progression of Parkinson’s disease [2]. In this field, the search for new imino-1,3-thiazinan-4-oneis a promising direction to design, develop and scale alternative electrochemical synthetic methodologie.

The convenient strategy is described for the conversion of *N*, *N*′-disubstituted thioureas and acryloyl chloride into the highly biologically valuable imino-1,3-thiazinan-4-one derivatives. The synthesis proceeds through a process with good yield promoted by an electrogenerated base (EGB) obtained with high current efficiency (scheme 1). In addition to this based on Structural Activity Relationship (SAR) studies, we have found suitable targets like G-protein coupled (CB1) cannabinoid receptor and Human 11beta-Hydroxysteroid Dehydrogenase Type 1 (11 βHSD1) for this synthesized molecule. The molecular docking studies were carried for our compound with CB1and 11 βHSD1 to understand the binding interaction mechanism and molecular dynamics simulations were performed to understand the stability of small molecule in CB1 and 11 βHSD1 microenvironment. Also, to understand the intermolecular stability Density Functional Theory (DFT) calculations were carried for free compound and compound in complex with CB1 and 11 βHSD1.



Scheme 1. Electrosynthesis of imino-1,3-thiazinan-4-one

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